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Jets and fragmentation

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Abstract. I review the status of next-to-leading-order calculations for hadronic final states in deeply-inelastic lepton–nucleon scattering. In more detail, I focus on calculations of (2+1)-jet-type cross sections, describe recent progress in extending the perturbative description into the transition region between deeply inelastic scattering and photoproduction, and study the validity of the fragmentation function picture for one-particle-inclusive cross sections at small Q^2 and small x_p.

1. Introduction

Recent experimental results from HERA at DESY show that the hadronic final state in deeply inelastic scattering can be studied with high precision. The results include the measurement of the strong coupling constant $\alpha_s(Q^2)$ by means of the (2+1)-jet rate $R_{2+1} = \sigma_{2+1}/\sigma_{\rm tot}$ [1, 2, 3] and event shapes [4], a direct determination of the gluon density [5], and the measurement of momentum fraction distributions for charged particles [6, 7]. The latter indicates that it may be possible to study scaling violations of fragmentation functions, the virtuality Q^2 of the photon being the relevant scale for the fragmentation process.

In this review I will concentrate on three selected topics:

- **NLO calculations for jet quantities:**
  To exploit the increased experimental precision reliable theoretical predictions in next-to-leading order (NLO) of QCD perturbation theory are required. In this proceedings contribution I give an overview of recent developments in NLO calculations for deeply-inelastic processes. The main improvement during the last two to three years was that universal Monte Carlo programs have become available which permit the numerical calculation of any (2+1)-jet-like infrared-safe observable in NLO.
- **Matching of DIS and photoproduction:**
  For photoproduction ($Q^2 \approx 0$) and deeply inelastic scattering (DIS, $Q^2 \gg \Lambda_{\rm QCD}$) it is well known how to calculate cross sections systematically in perturbation theory. Recently, a formalism [8, 9] has been developed which permits calculations in the transition region $Q^2 \sim \Lambda_{\rm QCD}$.

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- **One-particle-inclusive processes:**
  The measurements of momentum fraction distribution mentioned above show a very good agreement of experimental data and theoretical predictions in next-to-leading order for moderately large Q^2 and x_p. However, the theoretical prediction breaks down both for small Q^2 and small x_p.

For lack of space, I had to leave out many, if not most, interesting topics. For more detailed information, I would like to refer the interested reader to the proceedings of the DIS 98 workshop in Brussels [10].

2. NLO calculations for jet quantities

One of the basic problems of perturbative QCD calculations is that experimentally hadrons are observed in the final state while theoretical calculations yield results for partons. Moreover, not all observables can be calculated in perturbation theory in a meaningful way. In principle, there are two possibilities:

- *Infrared-safe observables*, which are constructed such that all soft and collinear singularities cancel among real and virtual corrections or can be absorbed into redefined parton densities. The same observable is then evaluated both for parton final states (theory prediction) and hadron final states (experimental data), possibly after the experimental data have been corrected for systematic errors.
- Alternatively, additional non-perturbative objects can be introduced, for instance *fragmentation functions*, which allow for a study of one-particle-inclusive processes. Fragmentation functions have to be measured and parametrized experimentally, and may serve to hide final-state collinear singularities which do not cancel because of integrations over restricted phase space regions.

In this section I consider the first possibility; one-particle-inclusive processes will be treated in Section 4.

In QCD perturbation theory, expectation values for parton observables are calculated as a phase space integral of a product of a differential parton cross section $\sigma^{(n)}(p_1,\ldots,p_n)$ for n-parton final states and an observable $\mathcal{O}^{(n)}(p_1,\ldots,p_n)$:

$$\langle\mathcal{O}\rangle = \sum_n \int \mathrm{dPS}^{(n)}\, \sigma^{(n)}(p_1,\ldots,p_n)\; \mathcal{O}^{(n)}(p_1,\ldots,p_n)\,. \tag{1}$$

In next-to-leading-order calculations, there are three contributions to be included:

$$\langle\mathcal{O}\rangle = \sigma_{\mathrm{Born}}\,\mathcal{O}^{(n-1)} + \sigma_{\mathrm{virtual}}\,\mathcal{O}^{(n-1)} + \sigma_{\mathrm{real}}\,\mathcal{O}^{(n)}. \tag{2}$$

Here σ_{Born} is the lowest order cross section, $\sigma_{\mathrm{virtual}}$ are the virtual and σ_{real} are the real corrections. If the Born term has $n-1$ final-state partons, $\sigma_{\mathrm{virtual}}$ will also have $n-1$ and σ_{real} will have n final-state partons. Infrared singularities arise in $\sigma_{\mathrm{virtual}}$ in the loop integrations and in σ_{real} in the phase space integration over $\mathrm{dPS}^{(n)}$.

As already mentioned in the introduction, theoretical predictions for partons in the final state are infrared-finite only for a special class of observables. The technical requirement for *infrared-safe observables* is that they behave well under soft and collinear limits:

$$\begin{aligned}
&\mathcal{O}^{(n)}(p_1,\ldots,p_i,\ldots,p_n) \underset{p_i\to 0}{\longrightarrow} \mathcal{O}^{(n-1)}(p_1,\ldots,\hat{p}_i,\ldots,p_n)\,, \\
&\mathcal{O}^{(n)}(p_1,\ldots,p_i,\ldots,p_j,\ldots,p_n) \underset{p_i\parallel p_j}{\longrightarrow} \mathcal{O}^{(n-1)}(p_1,\ldots,\hat{p}_i,\ldots,\hat{p}_j,\ldots,p_n,p_i+p_j)\,.
\end{aligned} \tag{3}$$

Momenta denoted by $\hat{p}$ are to be omitted.

The main technical problem is the extraction of the infrared singularities from the real corrections. It turns out that this can be done in an observable-independent way, such that it is possible to build Monte-Carlo programs which are able to integrate arbitrary infrared-safe observables. This can be done because the structure of QCD cross sections in kinematical limits is known: the factorization theorems of QCD [11] state that the structure of the parton cross section σ_{real} for collinear and soft limits is of the form of a product of a singular kernel K and the Born cross section $\sigma^{(n-1)}$:

$$\sigma^{(n)} \underset{\text{soft/collinear}}{\longrightarrow} K\,\sigma^{(n-1)}. \tag{4}$$

The product of σ_{real} and $\mathcal{O}^{(n)}$ thus behaves in a simple way: the cross section goes over into a kernel K and the Born cross section, and the observable approaches the corresponding observable for Born term kinematics. The kernel K is independent of the phase space variables of the $(n-1)$-particle phase space, and thus the phase space integration over the corresponding variables can be performed analytically.

2.1. Calculations

Particularly interesting for phenomenological applications are processes with 2+1 jets in the final state (which means that 2 jets are produced from the hard scattering cross section, plus the remnant jet of the incident photon). First of all, in leading order of QCD perturbation theory these processes are of $\mathcal{O}(\alpha_s)$, and are thus suitable for a measurement of the strong coupling constant α_s. Moreover, the gluon density enters in leading order in the so-called boson–gluon-fusion process. Therefore, this process can also be used to measure the gluon density [12, 13].

By now there are several calculations for (2+1)-jet processes available with corresponding weighted Monte-Carlo programs:

- `PROJET` [14]: The jet definition is restricted to the modified JADE jet clustering scheme; the program is based on the calculation published in Refs. [15, 16, 17].
- `DISJET` [18]: Again the jet definition is restricted to the modified JADE scheme; the program is based on the calculation in Refs. [19, 20].
- `MEPJET` [21]: This is a program for the calculation of arbitrary observables which uses the phase-space-slicing method. The corresponding calculation [22] uses the Giele–Glover formalism [23] for the analytical calculation of the IR-singular integrals of the real corrections, and the crossing-function technique [24] to handle initial-state singularities. The latter requires the calculation of "crossing functions" for each set of parton densities.
- `DISENT` [25]: This program is based on the subtraction method. The subtraction term is defined by means of the dipole formalism§ [26, 27].
- `DISASTER++` [28]: This is a `C++` class library‖ . The subtraction method is employed, and the construction of the subtraction term resembles the method

§ The subtraction term is written as a sum over dipoles (an "emitter" formed from two of the original partons and a "spectator" parton). Besides the factorization theorems of perturbative QCD, the main ingredient is an exact factorization formula for the three-particle phase space, which allows for a smooth mapping of an arbitrary 3-parton configuration onto the various singular contributions.

‖ The acronym stands for "Deeply Inelastic Scattering: All Subtractions Through Evaluated Residues". Most of the program is written in `C++`. A `FORTRAN` interface is available; thus there is no problem to interface the class library to existing `FORTRAN` code.

of Ref. [29], i.e. it is obtained by the evaluation of the residues of the cross section in the soft and collinear limits. Double counting of soft and collinear singularities is avoided by means of a general partial fractions method.

- `JetViP` [30]: This program implements the calculation of [31], which extends the previous calculations into the photoproduction limit $Q^2 \to 0$. The calculation has been done by means of the phase space slicing method. Up to now, the polarization of the virtual photon is restricted to be longitudinal or transverse.

The two basic approaches which are employed to extract the infrared singularities from the real corrections are the *phase-space-slicing method* and the *subtraction method*.

- The phase-space-slicing method splits up the full parton phase space into two regions: a region R where all partons can be resolved, and a region U where two or more partons are unresolved. This split is usually achieved by means of a technical cut parameter $s_{\min}$. Two partons with momenta p_1 and p_2 are unresolved if their invariant mass $2p_1p_2$ is smaller than $s_{\min}$ and resolved if it is larger. The integration over the resolved region R can be performed safely by Monte Carlo integration, because all infrared singularities are cut out by the phase space cut. The integration over the unresolved region U is divergent and cannot be performed numerically, but because of the constraint $2p_1p_2 < s_{\min}$ the cross section factorizes (see Eq. 4) in the limit $s_{\min} \to 0$. This contribution is *approximated* by this limit. The integration over the singular region can be done analytically, and the divergent parts can be extracted. In the limit of $s_{\min} \to 0$ the sum of the two integrals over R and U should approach the integral over the full phase space. It should be kept in mind that this convergence has to be checked explicitly by varying $s_{\min}$ and looking for a plateau in this variable.
- A calculation using the subtraction method defines a subtraction term S which makes the integral $\int \mathrm{dPS} \left(\sigma^{(n)} \mathcal{O}^{(n)} - S\right)$ finite. The original integral is, as an exact identity, rewritten as

$$\int \mathrm{dPS}\, \sigma^{(n)} \mathcal{O}^{(n)} = \int \mathrm{dPS} \left(\sigma^{(n)} \mathcal{O}^{(n)} - S\right) + \int \mathrm{dPS}\, S. \qquad (5)$$

  The first integral can be done by a Monte Carlo integration. For the term S, the factorization from Eq. 4 holds exactly. As for the phase-space-slicing method, the second term is integrated analytically. No technical cut-off has to be introduced¶.

Both methods have their merits and their drawbacks. The phase-space-slicing method is technically simple and can be easily implemented once the matrix elements for the real and virtual corrections are known. The main problem is the residual dependence on the technical cut $s_{\min}$. The independence of numerical results from variations of this cut has to be checked; moreover, the integration over the region R mentioned above requires very high statistics, because the integration region is close to the singular limit. The subtraction method does not require a technical cut, but the construction of the subtraction term S is usually quite involved. If this can be afforded, the subtraction method is the method of choice.

¶ This is, strictly speaking, not correct. A dimensionless cut t_{cut} of the order of 10^{-10} to 10^{-12} is used to avoid phase space regions where the subtraction no longer works because of the finite precision of floating point numbers.

2.2. Program comparisons

It is interesting to compare the available universal Monte Carlo programs numerically to check whether all available calculations are consistent. Experimental papers usually contain statements that the programs "agree on the one per cent level". A closer investigation, however, reveals that a statement of this kind is not correct. The three programs `MEPJET`, `DISENT` and `DISASTER++` have been compared in Ref. [28] for the modified JADE jet clustering algorithm in the E-scheme for several choices of physical and unphysical parton densities[+]. The result is that `DISENT 0.1` and `DISASTER++ 1.0` agree well, with discrepancies of the `MEPJET` results. Presently this is studied in the framework of the HERA Monte Carlo workshop[*] at DESY. There does not yet exist a systematic comparison of the `JetVip` program with `MEPJET`, `DISENT` and `DISASTER++`.

3. Matching of DIS and photoproduction

For large photon virtuality Q^2, the coupling of the exchanged virtual photon in a lepton–nucleon scattering process is exclusively pointlike. Extending this kind of calculation down to $Q^2 \approx 0$ leads to the problem that the photon propagator diverges. Instead, it is possible to calculate the scattering process for the scattering of a quasi-real photon and a nucleon, where the flux of quasi-real photons is described by a Weizsäcker–Williams approximation. For small Q^2, in addition to the cross section contribution from the pointlike coupling, a resolved contribution has to be added, because the quasi-real photon may fluctuate into a hadronic state, which in turn interacts strongly with the incident nucleon. This process is modelled by means of parton densities $f_{i/\gamma}$ of the virtual photon. The assumption of a photon structure is also required in order to treat collinear singularities arising from the splitting of the real photon via its pointlike coupling into a collinear quark-antiquark pair. This collinear singularity does not cancel against the virtual corrections, but is absorbed into the $f_{i/\gamma}$. Typically, the infrared singularities are regularized by dimensional regularization; the singularities then show up as poles in ϵ, where the space-time dimension is set to $d = 4 - 2\epsilon$.

This type of calculation has recently been extended to the case of exchanged photons with moderate Q^2 in Refs. [8, 9]. Here, because Q^2 is finite, strictly speaking there is no collinear singularity, and therefore no poles in ϵ related to the photon splitting arise. However, the integral over the phase space of the quark-antiquark pair yields a logarithm in Q^2. Because this logarithm may be large, and can therefore spoil perturbation theory, it has to be resummed. This is done by absorbing it into the redefined parton densities of the photon. The corresponding renormalization group equation then takes care of the resummation.

Depending on the factorization scale for the virtual photon, the resolved contribution can be surprisingly large even for fairly large Q^2, compared with the "standard" DIS calculation for the pointlike coupling. This seems to be in contradiction with the statement that the resolved contribution should die out for increasing Q^2. There are two reasons for this: (a) The choice of the factorization scale μ for the resolved photon dictates the size of the resolved contribution. The

[+] By "unphysical" I mean parton densities of the form $q(x) = (1-x)^\alpha$ and $g(x) = (1-x)^\alpha$, where α is some power. These are introduced to have a more stringent test on the hard scattering matrix elements.

[*] `http://home.cern.ch/~graudenz/heramc.html`

parton density of the virtual photon is exactly zero for $\mu = Q$. The factorization scale employed in Refs. [8, 9] is $\sqrt{Q^2 + E_T^2}$ (E_T is the transverse energy of the produced jets), which makes sure that even at large Q^2 there is always a resolved contribution. (b) In the full NLO calculation, there are four different matrix elements which contribute: the direct process in LO and NLO (with the dangerous logarithm in Q^2 subtracted), and the resolved process in LO and NLO. It is expected that the sum of the first three processes reproduce the result for the standard calculations, and this is indeed the case: the logarithm that has been subtracted for the direct coupling is added up again via the parton density of the photon in the LO resolved contribution. The difference comes from the resolved contribution in NLO: the corresponding parton subprocess, which is of $\mathcal{O}\left(\alpha_s^3\right)$, is one order in α_s higher than the "standard" calculation. Thus, this contribution could be considered as part of the NNLO correction to the Born term for (2+1)-jet production. Differences between the two approaches are therefore expected.

4. One-particle-inclusive processes

The comparison of x_p-distributions♯ for charged particle production from experimental data [6, 7] and the NLO program `CYCLOPS` [32, 33] leads to severe discrepancies for small values of Q^2 or small x_p. For large Q^2 and large x_p, data and theory agree nicely. Where does this discrepancy come from?

The theoretical prediction is made in the fragmentation function picture: the cross section for the inclusive production of charged particles is obtained by a convolution of the hard scattering cross section calculated in perturbative QCD and fragmentation functions which have been obtained from fits to e^+e^- data. Fragmentation functions depend on the momentum fraction z of the parent parton carried by the observed particle. An assumption in this picture is that the mass of the observed particle can be neglected relative to any other scale of the process, in particular relative to its momentum. The variable z can thus be defined either by means of fractions of energies or fractions of momenta. In the real world, the observed particle *has* a mass, and this gives, thus, rise to an uncertainty in the theoretical description. It is clear that mass effects will be important if $x_p = \mathcal{O}(2m_\pi/Q)$, m_π being a typical hadronic mass. It turns out that excluding data points with a value of x_p close to or smaller than this leads to a good agreement between data and theory. A different argument in terms of rapidities of partons and observed particles has been given in Ref. [34]. During the Durham workshop, a quantitative estimate of power corrections $\sim 1/Q^2$ to the fixed-order NLO prediction has been made. Y. Dokshitser and B. Webber proposed a factor $1/(1+4\mu^2/(x_pQ)^2)$, depending on a mass parameter μ, to be multiplied with the NLO cross section; this factor together with a fit of μ is able to describe the experimental data fairly well (see the contribution to these proceedings by P. Dixon, D. Kant, and G. Thompson).

5. Summary

I have discussed three topics related to hadronic final states at HERA. For the basic processes, theoretical predictions are available in next-to-leading-order accuracy.

♯ The variable x_p is defined to be the fraction $2E/Q$, where E is the energy of an observed particle in the current hemisphere of the Breit frame.

Independent calculations permit the comparison of results, and a few problems with Monte Carlo programs have already been fixed. What is still missing are calculations for W and Z-exchange in the subtraction formalism for jet cross sections. This is likely to become available in the near future. Moreover, a calculation for transverse momentum spectra of charged particles has not yet been done. The calculation for the transition region of DIS and photoproduction fills a gap in the theoretical description of lepton–nucleon scattering. However, it is not yet clear whether the parton densities for virtual photons are process-independent beyond NLO, such that they can be measured in one process and used for predictions in a different one. The necessity to introduce a power correction term for one-particle-inclusive distributions already at fairly large values of Q^2 shows that the calculation of fixed-order QCD corrections is not sufficient for a good description of experimental data. Unfortunately, a power correction term introduces an additional mass parameter, which cannot be calculated from first principles.

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7. References

[1] H1 Collaboration, preprints DESY 98–075, DESY 98–076, DESY 98–087 (June 1998).
[2] H1 Collaboration, Phys. Lett. **B346** (1995) 415.
[3] ZEUS Collaboration, Phys. Lett. **B363** (1995) 201.
[4] H1 Collaboration, Phys. Lett. **B406**(1997) 256.
[5] M. Hampel, *Measurement of the Gluon Density from Jet Rates in Deep Inelastic Scattering*, Doctoral thesis, preprint PITHA 97/13 (Aachen Univ., February 1997).
[6] H1 Collaboration, *Fragmentation Measurements in the Breit frame at HERA*, to appear in the proceedings of the 29th International Conference on High-Energy Physics, Vancouver, Canada, July 1998.
[7] ZEUS Collaboration, Z. Phys. **C70** (1996) 1, Phys. Lett. **B414** (1997) 428.
[8] G. Kramer, B. Pötter, Eur. Phys. J. **C5** (1998) 665.
[9] M. Klasen, G. Kramer, B. Pötter, Eur. Phys. J. **C1** (1998) 261.
[10] Proceedings of the 6th International Workshop on Deep Inelastic Scattering and QCD (Brussels 1998); see also `http://asrv1.iihe.ac.be/dis98/`.
[11] J.C. Collins, D.E. Soper and G. Sterman, in: *Perturbative Quantum Chromodynamics*, ed. A.H. Mueller, World Scientific (Singapore, 1989).
[12] D. Graudenz, M. Hampel, A. Vogt and Ch. Berger, Z. Phys. **C70** (1996) 77.
[13] D. Graudenz, M. Hampel and A. Vogt, in: Proceedings of the workshop on future physics at HERA, eds. G. Ingelman, A. De Roeck, R. Klanner (Hamburg 1995/96).
[14] D. Graudenz, Comput. Phys. Commun. **92** (1995) 65.
[15] D. Graudenz, *The three-jet cross section at order α_s^2 in deep-inelastic electron–proton scattering*, Doctoral thesis (September 1990).
[16] D. Graudenz, Phys. Lett. **B256** (1991) 518.
[17] D. Graudenz, Phys. Rev. **D49** (1994) 3291.
[18] T. Brodkorb and E. Mirkes, `DISJET` *program manual*, preprint MAD/PH/821 (Madison 1994).
[19] T. Brodkorb and J.G. Körner, Z. Phys. **C54** (1992) 519.
[20] T. Brodkorb and E. Mirkes, Z. Phys. **C66** (1995) 141.
[21] E. Mirkes and D. Zeppenfeld, `MEPJET 2.0` *program manual*, unpublished (1997).
[22] E. Mirkes and D. Zeppenfeld, Phys. Lett. **B380** (1996) 205.
[23] W.T. Giele and E.W.N. Glover, Phys. Rev. **D46** (1992) 1980.

[24] W.T. Giele, E.W.N. Glover and D.A. Kosower, Nucl. Phys. **B403** (1993) 633.
[25] S. Catani and M. Seymour, `DISENT 0.0` *program manual*, unpublished (1996).
[26] S. Catani and M. Seymour, in: Proceedings of the workshop on future physics at HERA, eds. G. Ingelman, A. De Roeck, R. Klanner (Hamburg 1995/96).
[27] S. Catani and M. Seymour, Nucl. Phys. **B485** (1997) 291.
[28] D. Graudenz, `DISASTER++` *version 1.0.1 program manual*, preprint `hep-ph/9710244` (December 1997).
[29] Z. Kunszt and D.E. Soper, Phys. Rev. **D46** (1992) 192.
[30] B. Pötter, `JetViP 1.1` *program manual*, preprint DESY 98-071 (June 1998).
[31] B. Pötter, preprint DESY 98-052 (June 1998).
[32] D. Graudenz, Phys. Lett. **B406** (1997) 178.
[33] D. Graudenz, `CYCLOPS` *(Monte Carlo program for one-particle-inclusive processes),* `http://home.cern.ch/~graudenz/cyclops_v1.2.uu`.
[34] D. Graudenz, *Deeply Inelastic Hadronic Final States: QCD Corrections*, in: Proceedings of the workshop on new trends in HERA physics, Ringberg castle, May 1997.